

DMRG Simulation of the SU(3) AFM Heisenberg Model

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We analyze the antiferromagnetic SU(3) Heisenberg chain by means of the Density Matrix Renormalization Group (DMRG). The results confirm that the model is critical and the computation of its central charge and the scaling dimensions of the first excited states show that the underlying low energy conformal field theory is the SU(3)₁ Wess-Zumino-Novikov-Witten model.

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I. INTRODUCTION

In recent years, a renewed interest in models of condensed matter with a symmetry larger than SU(2) has arisen. This is because these models represent not only challenging theoretical problems but also can be effectively implemented experimentally. In particular SU(4) systems can be realized in laboratories in transition metals oxides [1] where the electron spin is coupled to the orbital degrees of freedom. A possible realization of SU(3) antiferromagnetic (AFM) spin chains in systems of ultra-cold atoms in optical lattices has been recently proposed [2]. In this case the spin would be related to the SU(3) rotation in an internal space spanned by the three available atomic states (colors, in the SU(3) language), with the condition that the number of particles of each color is conserved. Other examples involve the SU(3) trimer state in a spin tetrahedron chain [3, 4], or the spin tube models in a magnetic field [5] where the low-energy effective Hamiltonian can be identified with a particular anisotropic SU(3) spin chain.

From a theoretical point of view, the SU(3) spin model has also been studied from different viewpoints. In recent years the interest on ferromagnetic SU(N) spin chains has been boosted by their implication in the AdS/CFT correspondence [6, 7]. On the other side the family of integrable spin chains include some models with SU(3) symmetry, as first shown by Sutherland [8], who generalized the Bethe-Ansatz to multiple component systems which include the SU(3) spin chain, showing that it is gapless. Also the SU(3) Heisenberg model can be di-

rectly related to a particular SU(3)-symmetric bilinear biquadratic spin-1 chain, the Lai-Sutherland (LS) model, which is also known to be critical [9, 10]. In terms of Conformal Field Theory (CFT) the LS model and the SU(3) spin chain should belong to the same universality class, that of the SU(3)₁ Wess-Zumino-Novikov-Witten (WZNW) model [11, 12].

In this paper we present a numerical analysis of the SU(3) spin chain by means of the Density Matrix Renormalization Group (DMRG). After a short description of the model and its mathematical framework (Section II), we present our new results (Section III) which confirm the criticality of the model as well as its correspondence to the Lai-Sutherland model. In particular, due to the ability of our program to provide the quantum numbers for each state, we can show that the excited states of the spin chain have the same quantum numbers as the irreducible representations (IR) of SU(3). We compute the scaling dimensions of the first excitations which turn out to agree with those of the SU(3)₁ WZNW model which corresponds to the low energy effective field theory descriptions of our spin chain. The results are further confirmed by the computation of the central charge by means of the vacuum entanglement entropy.

II. THE SU(3) MODEL

We consider the following Heisenberg model

$$H = J \sum_{i=1}^L \mathbf{S}_i \cdot \mathbf{S}_{i+1} \quad (1)$$

where the spin variables are expressed in terms of the generators of SU(3) in the fundamental representation:

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$\mathbf{S}_i^a = \frac{1}{2}\lambda_i^a$, with $a = 1, \dots, 8$ and λ_a the eight Gell-Mann matrices. The sign of J selects respectively an antiferromagnetic spin chain ($J > 0$) or a ferromagnetic (FM) one ($J < 0$). In the following we shall concentrate only on the AFM case, which has been partially considered also in ref. [13, 14].

In terms of the following ladder operators, $T^\pm = \lambda^1 \pm i\lambda^2$, $V^\pm = \lambda^4 \pm i\lambda^5$ and $U^\pm = \lambda^6 \pm i\lambda^7$, the Hamiltonian (1) becomes

$$H = \frac{J}{2} \sum_{i=1}^L \left\{ \frac{1}{4} (T_i^+ T_{i+1}^- + V_i^+ V_{i+1}^- + U_i^+ U_{i+1}^- + h.c.) + \frac{1}{2} \lambda_i^3 \lambda_{i+1}^3 + \frac{1}{2} \lambda_i^8 \lambda_{i+1}^8 \right\}. \quad (2)$$

This makes easier to identify two operators, S_z and Q_z , given by the sums of the two diagonal Gell-Mann matrices

$$S_z = \sum_i \frac{1}{2} \lambda_i^3 \quad Q_z = \sum_i \frac{\sqrt{3}}{2} \lambda_i^8, \quad (3)$$

that commute with the Hamiltonian and correspond to conserved quantities (isospin and hypercharge). The corresponding quantum numbers label the different eigenstates of (1).

The Lai-Sutherland model is defined as the bilinear biquadratic spin-1 chain

$$H = J' \sum_{i=1}^L \left[\tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1} + (\tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1})^2 \right], \quad (4)$$

and characterized by an $SU(3)$ symmetry. The model (4) and the $SU(3)$ spin chain can be mapped one onto the other by means of the following identity [15]

$$\tilde{\mathbf{S}}_i \tilde{\mathbf{S}}_{i+1} + (\tilde{\mathbf{S}}_i \tilde{\mathbf{S}}_{i+1})^2 - 1 = \frac{1}{3} + \frac{1}{2} \sum_{a=1}^8 \lambda_i^a \lambda_{i+1}^a. \quad (5)$$

We have already mentioned in the introduction that the LS model is known to be gapless and to belong to the same universality class of the $SU(3)$ level-1 Wess-Zumino-Novikov-Witten model with central charge $c = 2$. Due to the correspondence between the two models, the $SU(3)_1$ WZNW model has to be the low energy effective critical field theory also for the $SU(3)$ spin chain. We shall numerically show that the $SU(3)$ Heisenberg chain is critical, and from the energy state obtained from the DMRG, we shall compute the central charge and the scaling dimensions of (1) and compare them to the values predicted for the $SU(3)_1$ WZNW model.

The states of the spin chain can be organized according to the irreducible representations of the affine (Kac-Moody) Lie algebra associated to $SU(3)$. Let us recall [16] that a useful way of representing the IR's of the Lie

λ	$\bar{\lambda}$	(S_z, Q_z)	$x_{\lambda, \bar{\lambda}}$
(1)	(1)	(0,0)	0
(3)	(1)	$\left\{ \begin{array}{l} (\pm 1/2, 1/2) \\ (0, -1) \end{array} \right\}$	1/3
($\bar{3}$)	(1)	$\left\{ \begin{array}{l} (\pm 1/2, -1/2) \\ (0, 1) \end{array} \right\}$	1/3
(3)	($\bar{3}$)	$\left\{ \begin{array}{l} (\pm 1/2, \pm 3/2) \\ (0, 0) \text{ (3 times)} \\ (\pm 1, 0) \end{array} \right\}$	2/3

Table I: Quantum numbers and scaling dimensions for some of the primary fields $\Phi_{\lambda, \bar{\lambda}}$ of the $SU(3)_1$ WZNW model.

algebra $su(3)$ is through the Young Tableau (YT) which can be labelled by two positive integer numbers (p, q) . Once p and q are known, one can easily compute the dimension d of the representation and the quantum numbers associated to the isospin S_z and the hypercharge Q_z according to [16, 17]:

$$d = \frac{1}{2}(p+1)(q+1)(p+q+2) \quad (6)$$

and

$$S_z = -I, -I+1, \dots, I-1, I \quad (7)$$

$$Q_z = \frac{3}{2}Y$$

where $I = \frac{1}{2}(r+s)$ and $Y = (r-s) - \frac{2}{3}(p-q)$, with $0 \leq r \leq p$, $0 \leq s \leq q$. In particular, the cases (1,0) and (0,1) give respectively the fundamental (**3**) and the anti-fundamental ($\bar{\mathbf{3}}$) IR, while the singlet representation (1) corresponds to (0,0).

It has been proved [18] that, in analogy with the $SU(2)$ case, the ground state (GS) of the AFM $SU(3)$ Hamiltonian is a singlet and, since it is made of particles u , d and s in equal number, it can be obtained in finite chains having only a number of sites which is a multiple of three, $L = 3M$. As for the excited states, we expect them to be in correspondence with the tower of conformal states of the corresponding $SU(3)$ WZNW model. The primary states of this theory are a finite number and are given [16] by fields $\Phi_{\lambda, \bar{\lambda}}$, whose holomorphic (antiholomorphic) part transforms according to a representation $\lambda = (p, q)$ ($\bar{\lambda} = (p', q')$) with the values of p, q (and similarly of p', q') satisfying the condition: $p+q \leq k$, k being the level. The conformal dimension of the primary field is then $x_{\lambda, \bar{\lambda}} = x_{(p, q)} + x_{(p', q')}$ with

$$x_{(p, q)} = \frac{1}{3(k+N)}(p^2 + q^2 + pq + 3p + 3q), \quad (8)$$

and a similar expression for $x_{(p', q')}$. For future reference, the values of $x_{\lambda, \bar{\lambda}}$ for some primary fields in the case of $k = 1$ are reported in Table I.

To end up this section, we notice that in a finite chain of length L not all quantum numbers, i.e. states, may be realized. For examples, working with periodic boundary

conditions and with an even number of sites, the singlet $(\mathbf{1}) \times (\mathbf{1})$ (ground) state, with $x = 0$, appears only for chains with $L = 6M$ (with M a positive and integer number), while the $(\mathbf{3}) \times (\mathbf{1})$ (or the $(\mathbf{1}) \times (\mathbf{\bar{3}})$) states are present only if $L = 6M + 4$ (or $L = 6M + 2$), both with $x = 1/3$.

III. NUMERICAL ANALYSIS

The SU(3) version of the DMRG we have used implements the following Hamiltonian

$$H = \frac{J}{2} \sum_{i=1}^L \left[\frac{1}{4} (k_0 T_i^+ T_{i+1}^- + k_1 V_i^+ V_{i+1}^- + k_2 U_i^+ U_{i+1}^- + h.c.) + \frac{1}{2} (z_0 \lambda_i^3 \lambda_{i+1}^3 + z_1 \lambda_i^8 \lambda_{i+1}^8) \right] \quad (9)$$

where k_j and z_j are input parameters. The model (9) reproduces the AFM (FM) case when all the k_j 's and the z_j 's are equal to 1 (-1). By tuning the input parameters k_j and z_j , we can study all the possible anisotropic version of the SU(3) Heisenberg model. A very important feature of this DMRG is that it implements both the quantum numbers S_z and Q_z given in (3). This implementation considerably reduces the computation time and, on the other hand, once S_z and Q_z are fixed from input, each run of the DMRG yields exclusively the energies of the states within those quantum-number sectors. This is very useful when one needs to classify the excitations according to the values of the isospin and of the hypercharge.

By setting $k_1 = k_2 = z_1 = 0$, we restrict to the SU(2) sector of SU(3). This has been used as a check to the program; the DMRG in this case reproduces perfectly all the energy states of the SU(2) Heisenberg model.

We study now the isotropic AFM chain with periodic boundary conditions by means of an infinite size DMRG with up to $m = 2200$ states in order to reduce the uncertainty on the energies to the order of magnitude of the truncation error. The data for the ground state and the first excited states are plotted in Fig. 1.

Let us first concentrate on the *ground state*, which, in agreement with theoretical predictions, it is found only when $L = 6M$. The plot of E_{00} as a function of $1/L^2$ shows a good linear behavior; this justifies the fitting of our data by the CFT equations for the GS:

$$\frac{E_{00}}{L} = e_\infty - \frac{\pi cv}{6L^2}, \quad (10)$$

where e_∞ and the product cv are kept as fitting parameters. We obtain: $e_\infty = -0.518288$ and $cv = 2.04419$. In order to derive the value of v we need an independent derivation of c . The central charge for a SU(N) level- k WZNW model is given by [16]

$$c = \frac{k(N^2 - 1)}{k + N}. \quad (11)$$

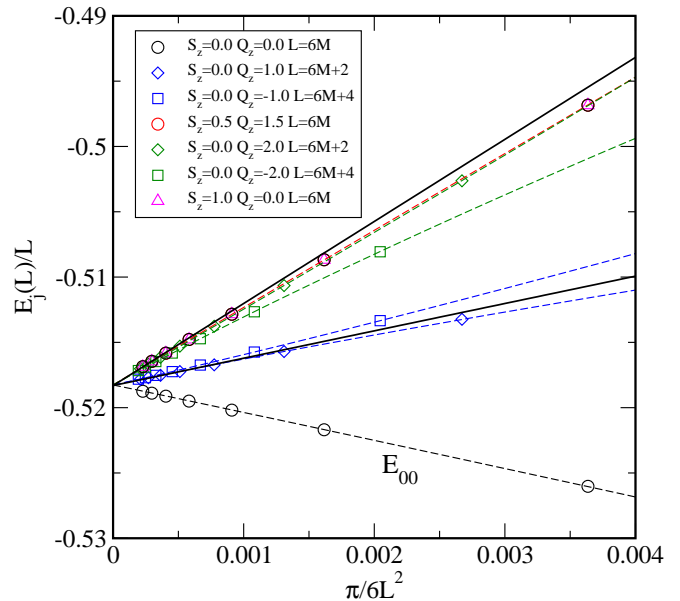


Figure 1: Plot of the ground state E_{00} and of the excited states for chains of different lengths (from $L = 12$ up to $L = 52$). The solid lines have a slope respectively of $\frac{1}{3}$ and $\frac{2}{3}$ and have been drawn as a guide for the eye. For sake of clarity, not all the degeneracies have been reported.

If the effective field theory describing our spin chain is the conformal $SU(3)_1$ WZNW model, the central charge must be $c = 2$.

However, it is possible to have a direct numerical derivation of c from the asymptotic behavior of the von Neumann entropy $S_n = -\text{Tr}_n(\rho_n \log_2 \rho_n)$ of the reduced density matrix $\rho_n = \text{Tr}_{i>n} \rho$ of a subchain with n spins of a critical system of length L , as a function of n and L , where ρ is the density matrix associated to the ground state of the chain. Indeed, one has [19, 20]:

$$S_n = \frac{c}{3} \log_2 \left[\frac{L}{\pi} \sin \left(\frac{\pi n}{L} \right) \right] + A. \quad (12)$$

As usual c is the central charge while A is a non-universal constant. The DMRG computes the density matrix for a block of length n in a chain of length L , so that S_n becomes quite simple to calculate. Fig. 2 shows the behavior of the von Neumann entropy as a function of the block length n in (a) and as a function of the quantity $y = \log_2 \left(\frac{L}{\pi} \right) / 3$ (obtained from (12) by setting $n = L/2$) in (b), for values of the DMRG states equal to 1000 and 2000. The data confirm the linear behavior expected from Eq. (12). The linear regression $S_n = cy + A$ yields the value for the constant $A = (1.774 \pm 0.002)$ and for the central charge $c = (1.995 \pm 0.001)$. Thus the theoretical prediction of Eq. (11) is confirmed with very high accuracy. From Fig. 2(b) it is also evident that the values obtained when keeping only 1000 states in the DMRG run are much less precise. This is the reason why we have then performed all calculations while keeping 2000

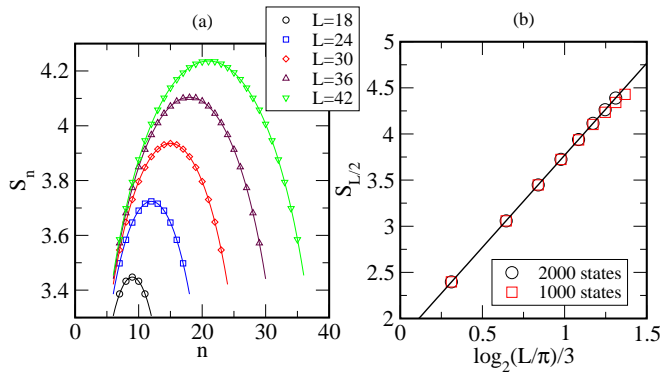


Figure 2: Analysis of the von Neumann entropy. The figure on the left (a) shows S_n for $m = 1000$ DMRG states as a function of the block length n for different chains of length L ; the figure on the right (b) is the plot of the half chain entropy ($n = L/2$) for $m = 1000$ and $m = 2000$ DMRG states. The linear fit on these data provides the values for the central charge c and the constant A .

states. Finally, the value of c can be substituted into the product cv derived from the GS to recover the velocity of the excited modes: $v = (1.0247 \pm 0.0005)$, which is close to the expected value [8] $\pi/3$.

Before proceeding with the analysis of the excited states, let us check the asymptotic value of the energy density e_∞ . The theoretical prediction for the ground state of the $S = 1$ bilinear biquadratic Heisenberg Hamiltonian (see Ref. [21]) is

$$E_{GS} = -\ln 3 - \frac{\pi}{3\sqrt{3}} + 1, \quad (13)$$

which already takes into account the factor -1 of the l.h.s. of equation (5). Starting from the correspondence between our $SU(3)$ chain and the biquadratic one (5), we can compare the value of e_∞ we obtained with the one predicted by equation (13): $E_{GS} = -0.703212$. The match is exact to the third decimal (-0.703243), if one also recalls that the Hamiltonian has a factor $1/4$ (due to the definition of the spin variables in terms of the $SU(3)$ generators) so that e_∞ needs to be multiplied by a factor two, and summed to the factor $1/3$ of equation (5). This is a further numerical proof of the equivalence between the the Lai-Sutherland and the $SU(3)$ spin model.

Let us study now the *excited states*. From Fig. 1, one immediately sees that the slope of excited states depends on the length of the chain. In particular, for $L = 6M$ the first excitation scales with a slope which is unmistakably different from the slope of the $L = 6M+2$ or $L = 6M+4$ data. For small values of L the data corresponding to the same S_z but with opposite Q_z are split by a finite size correction, while for increasing values of L they tend to overlap and scale to the same asymptotic value.

For the excited states CFT predicts that:

$$E_j - E_{00} = \frac{2\pi v}{L} x_j \quad (14)$$

L	x_1	x_2
$6M+2$	0.3414 ± 0.0001	0.6291 ± 0.0003
$6M+4$	0.3406 ± 0.0002	0.6238 ± 0.0003
(\blacktriangle)	0.3410 ± 0.0002	0.6265 ± 0.0003
$6M$	-	0.6503 ± 0.0003

Table II: Results of the numerical analysis. The velocity and the central charge are respectively: $v = (1.0247 \pm 0.0005)$ and $c = (1.995 \pm 0.001)$. The scaling dimensions of the first (x_1) and the second (x_2) excited states for each L are calculated as described in the text. The mean value (\blacktriangle) between $L = 6M+2$ and $L = 6M+4$ for x_1 and x_2 is provided (see also Fig. 1). For $L = 6M$ only the first excitation above the ground state has been considered.

where x_j is the scaling dimension of the j -th excitation for a given chain of length L ; E_{00} is given by Eq. (10) where c and v have been derived before and are reported in the caption of Table II. The numerical coefficients for the scaling dimensions that one can obtain from the DMRG data of Fig. 1 are listed in Table II.

As expected, the values of the allowed conformal dimensions are very close to the values of $1/3$ and $2/3$ predicted by a $SU(3)_1$ WZNW model.

IV. CONCLUSIONS

We have provided strong numerical evidence of the criticality of the AFM $SU(3)$ spin chain. Also, we have confirmed that the conformal field theory describing the chain is effectively the $SU(3)_1$ WZNW model, by computing the central charge and scaling dimensions of the lowest excited states of the model, which turn out to be organized according to the IR of $SU(3)_1$ Kac-Moody algebra.

There are many interesting generalizations of the above models which deserve further study. In particular, a similar ferromagnetic spin chain is connected with the non-linear CP^2 sigma mode at $\theta = \pi$ and might be useful to clarify some controversial problems of the model. Another interesting problem is to consider larger $SU(N)$ symmetry groups. In two-dimensional chains, the vacuum state is of Néel type for $N \leq 4$ and of Spin-Peierls type for $N \geq 5$ [22]. The analysis by means of DMRG technique might shed some light on the transition mechanism.

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